EM-0

$\boxed{\text{Electric Fields in Matter}}$

At the heart of Condensed Matter physics

You can see why $\vec{j} = \sigma \vec{E}$ $\quad (I = V/R)$

conductivity

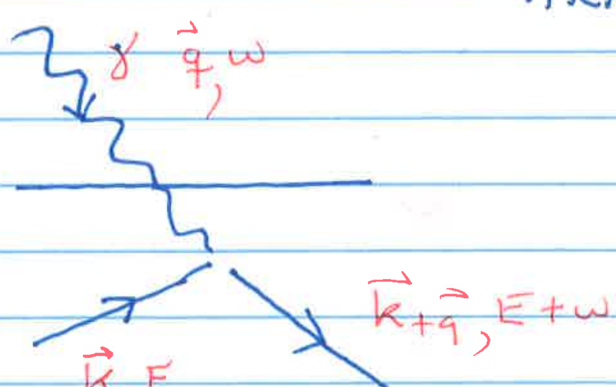
Not just static

$\vec{E}(\vec{q},\omega)$ $\quad \vec{B}(\vec{q}\,\omega)$ $\quad \leftarrow$ EM waves (light)

$\sigma(\vec{q},\omega)$ determines whether solid is transparent or opaque (ω dependent statement)

Treat light as photons

ARPES {

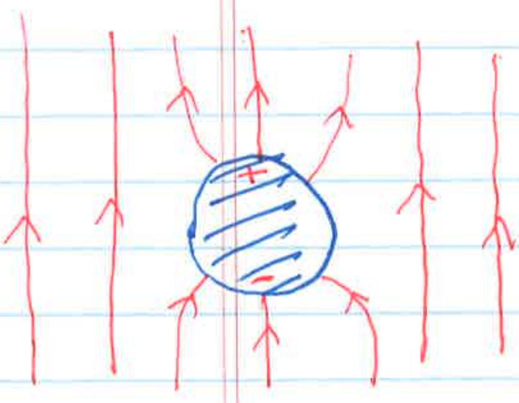


Infer knowledge of dispersion relations $E(\vec{k})$ from absorption of photons

EM-1

Electric Fields in Matter

Already got a start on this problem



$$\vec{E} = -\vec{\nabla} V$$

$$V(r,\theta) = -E_0\left(r - R^3/r^2\right)\cos\theta$$

induced dipole field

$\frac{1}{4\pi\epsilon_0}\frac{\vec{p}\cdot\hat{r}}{r^2}$ $\vec{p}$ is in $\hat{z}$ direction

$$|\vec{p}| = E_0 R^3 \frac{1}{4\pi\epsilon_0}$$

Conducting sphere in uniform $\vec{E} = E_0\hat{z}$

In general $\vec{p} = \alpha\vec{E}$

polarizability

$\frac{\alpha}{4\pi\epsilon_0}$ units: Volume

EM-2

Model atom as point charge q (proton) at origin and uniform spherical cloud of charge $-q$ (electrons) and radius a around it.

Apply $\vec{E}$: proton + spherical clouds displaced by d

proton equilibrium: (assume e^- cloud stays spherical)

$$\underbrace{qE}_{\text{external field}} = \underbrace{q \frac{1}{4\pi\epsilon_0} \frac{q}{\frac{4}{3}\pi a^3}}_{\text{electrons attract}} \frac{4}{3}\pi d^3 \frac{1}{d^2}$$

$$E = \frac{1}{4\pi\epsilon_0} qd/a^3$$

$$p = qd = \underbrace{(4\pi\epsilon_0 a^3)}_{\alpha} E$$

	$\alpha/4\pi\epsilon_0$ $(10^{-30}\ m^3)$
H	0.667
He	0.205
Li	24.3
Be	5.6
C	1.67
Ne	0.396

volumes decrease? Is this true

Bohr radius $a_0 = 0.5\ \mathring{A}$
$= 0.5\ 10^{-10}\ m$

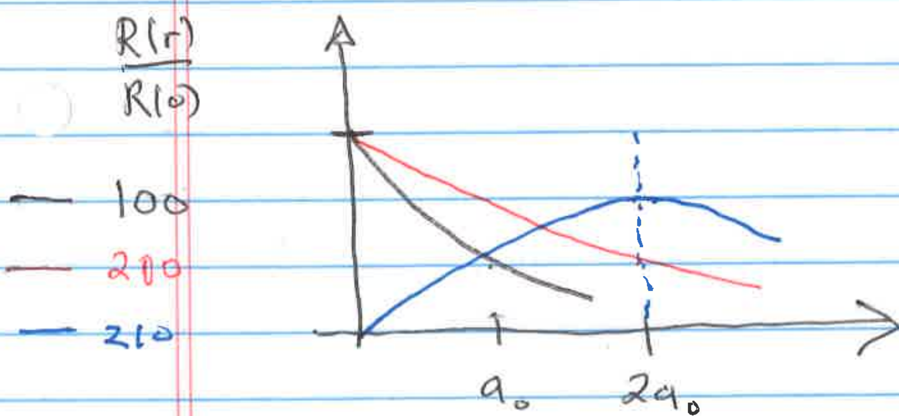
$a_0^3 = 0.13 \cdot 10^{-30}$

EM-2A

Bohr radius a_0

Hydrogen atom wave functions

n	l	m	F(ϕ)	P(θ)	R(r)
1	0	0	$1/\sqrt{2\pi}$	$1/\sqrt{2}$	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$
2	0	0	$1/\sqrt{2\pi}$	$1/\sqrt{2}$	$\frac{2}{2\sqrt{2}\, a_0^{3/2}}(2 - r/a_0)\, e^{-r/2a_0}$
2	1	0	$1/\sqrt{2\pi}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}} \frac{1}{a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$
2	1	±1	$1/\sqrt{2\pi}\, e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}} \frac{1}{a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$



⟹ P should increase across periodic table row ?!

Q: what are we missing?

Charge Z on nucleus

$$e^{-Zr/2a_0}$$

n=2 completes second row

But Z goes up to 8

and wins!

EM-2B

$P(r) \sim \underset{\substack{\uparrow \\ \text{phasespace}}}{r^2} e^{-r/b}$ $\qquad b = n/z$

assuming no θ, ϕ dependence

$$\int_0^\infty \underbrace{r^2}_{u} \underbrace{e^{-r/b} dr}_{dv} = -br^2 e^{-r/b}\Big|_0^\infty + b\int_0^\infty 2re^{-r/b} dr$$

$$= 2b\left\{ re^{-r/b}\Big|_0^\infty + b\int_0^\infty e^{-r/b} dr \right\}$$

$$= 2b^3$$

$$\langle r \rangle = \frac{1}{2b^3}\int_0^\infty r^3 e^{-r/b} dr = \frac{1}{2b^3} 6b^4 = 3b$$

$$\langle r \rangle = 3n/z$$

Predict size falls by $3/10$ factor Li to Ne

Li $z = 3$

Ne $z = 10$

$\propto \sim$ Volume $\sim$

$(3/10)^3 = 27/1000$

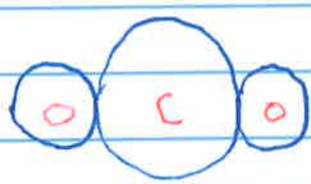
$= .0027$

Actual $\frac{0.396}{24.3} = .0162$

EM-3

Molecules trickier: Shape may cause easier polarization along one direction than another

CO_2



$$\vec{p} = \alpha_\perp E_\perp$$

$$\alpha_\perp = 2 \cdot 10^{-40} \frac{C^2 m}{N}$$

$$\frac{\alpha_\perp}{4\pi\epsilon_0} = 1.8 \cdot 10^{-30} m^3$$

$$\vec{p} = \alpha_{\parallel} \vec{E}_{\parallel}$$

$$\alpha_{\parallel} = 4.5 \cdot 10^{-40} \frac{C^2 m}{N}$$

$$\frac{\alpha_{\parallel}}{4\pi\epsilon_0} = 4.0 \cdot 10^{-30} m^3$$

CO_2 is simple since linear

Even uglier:

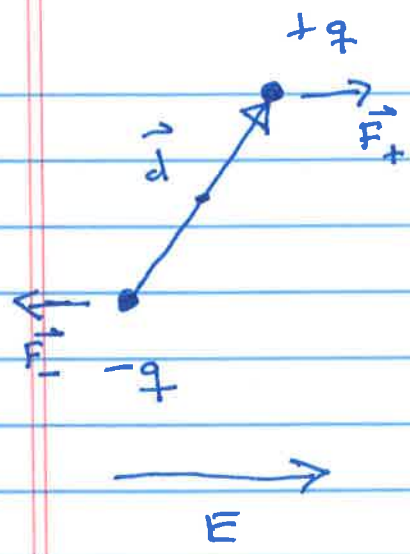
$$p_x = \alpha_{xx} E_x + \alpha_{xy} E_y + \alpha_{xz} E_z$$

$$p_y =$$

$$p_z =$$

$$\alpha_{ij} \equiv \text{polarizability tensor}$$

EM-4



$\vec{F}_{tot} = 0$ but torque nonzero

$$\vec{\tau} = \frac{\vec{d}}{2} \times q\vec{E} + \left(-\vec{d}/2\right) \times \left(-q\vec{E}\right)$$

$$= q\vec{d} \times \vec{E} = \vec{p} \times \vec{E}$$

EM-5

Single dipole

$$V(r) = \frac{1}{4\pi\epsilon_0} \frac{\vec{p}\cdot\hat{r}}{r^2}$$

dipole "density"

$\vec{P}(r')\,d\tau'$ dipole in volume $d\tau'$

Many dipoles

$$V(r) = \frac{1}{4\pi\epsilon_0} \int \frac{P(r')\cdot\hat{\mathcal{R}}}{\mathcal{R}^2}\, d\tau'$$

$\vec{\mathcal{R}}$ here really $\vec{r}-\vec{r}'$

$$\vec{\nabla}'\left(\frac{1}{\mathcal{R}}\right) = \frac{\hat{\mathcal{R}}}{\mathcal{R}^2}$$

$$V(r) = \frac{1}{4\pi\epsilon_0} \int \vec{P}\cdot\vec{\nabla}'\frac{1}{\mathcal{R}}\, d\tau'$$

$$= \frac{1}{4\pi\epsilon_0}\left\{\int \vec{\nabla}'\cdot\left(\frac{\vec{P}}{\mathcal{R}}\right) d\tau' - \int \frac{1}{\mathcal{R}}(\nabla'\cdot P)\,d\tau'\right\}$$

$$= \frac{1}{4\pi\epsilon_0} \int_S \underbrace{\frac{1}{\mathcal{R}}\vec{P}\cdot d\vec{a}'} - \frac{1}{4\pi\epsilon_0}\int \frac{1}{\mathcal{R}}(\vec{\nabla}'\cdot\vec{P})\,d\tau'$$

$\sigma_b \equiv \vec{P}\cdot d\vec{a}'$

potential due to $\rho_b = -\vec{\nabla}'\cdot\vec{P}$

precisely the form of potential due to charge on a surface

if we define

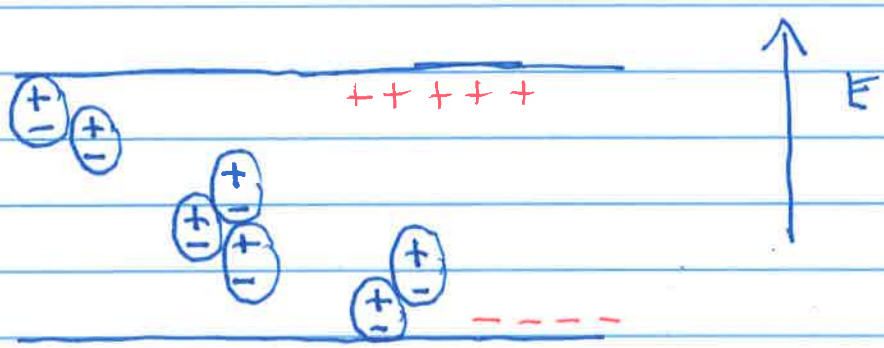
Potential (and field) of polarized object

$\equiv$ Same as $\rho_b = -\vec{\nabla}\cdot\vec{P}$ "bound charges"

$\sigma_b \equiv \vec{P}\cdot\hat{n}$

EM-6

Physical picture infinite slab



cancels in interior only charge at surface

Pickett's "polarization catastrophe" PRL 102 107602 (2009)

$\longrightarrow$ EM6A

Uniformly polarized sphere. $\vec{\nabla}\cdot\vec{P} = 0$

$\uparrow$ uniform

$$\sigma_b = \vec{P}\cdot\hat{n} = P\cos\theta$$

$$V(r,\theta) = \frac{P}{3\epsilon_0}\, r\cos\theta \qquad r < R$$

$$\frac{P}{3\epsilon_0}\,\frac{R^3}{r^2}\cos\theta \qquad r > R$$

"usual" argument eg from HW! r^ℓ, $r^{-(\ell+1)}$ $P_\ell(\cos\theta)$

EM6A

If no internal cancellation..

Heterostructure Polar $LaAlO_3$ ← LaO (+) charge ← AlO_2 (−) charge

+ nonpolar $SrTiO_3$

⇒ "Ever increasing dipole"

AlO_2^- $-\sigma$

LaO^+ $+\sigma$

AlO_2^- $-\sigma$ ϕ

$\uparrow E$

LaO^+ $+\sigma$ ⇒ potential grows indefinitely

ϕ

AlO_2^- $-\sigma$

$\uparrow E$

LaO^+ $+\sigma$

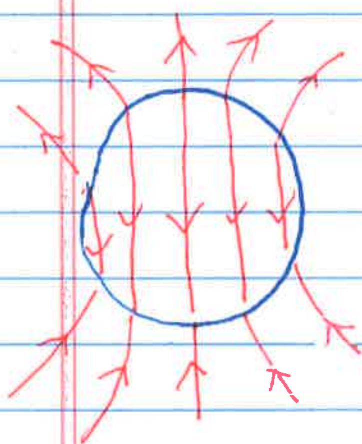
$SrTiO_3$ surface

EM-7

$\vec{E} = -\vec{\nabla} V$ inside $V = \frac{P}{3\epsilon_0} z$

and $E = -\vec{P}/3\epsilon_0$

outside $V = \frac{1}{4\pi\epsilon_0} \frac{\vec{p} \cdot \hat{r}}{r^2}$ $p = \frac{4}{3}\pi R^3 P$



Weird? not really : Picture

$\sigma_b = \vec{P} \cdot \hat{n}$ on surface

$\theta = 0$ $\vec{p} \cdot \hat{r} = P$

along $\hat{z}$ axis $V = \frac{1}{4\pi\epsilon_0} \frac{P}{r^2} = \frac{1}{4\pi\epsilon_0} \frac{P}{z^2}$

$\vec{E} = -\vec{\nabla} V = P/2\pi\epsilon_0 z^3 \, \hat{z}$

$\theta = \pi$ $\vec{p} \cdot \hat{r} = -p$ $V = -\frac{1}{4\pi\epsilon_0} P/z^2$

$E = -\vec{\nabla} V = \underbrace{-P/2\pi\epsilon_0 z^3}_{>0 \text{ since } z<0} \, \hat{z}$

EM8

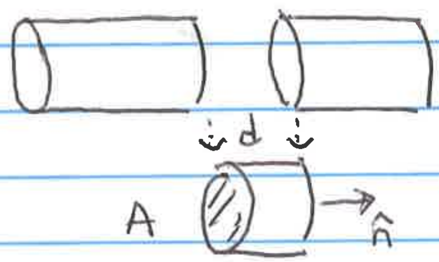
Electric field of collection of dipoles can be interpreted in terms of "bound" charge

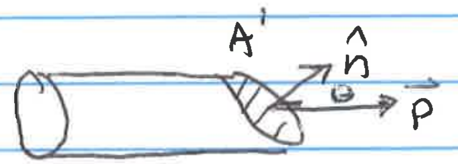
$$\sigma_b = \vec{P}\cdot\hat{n} \qquad \rho_b = -\vec{\nabla}\cdot\vec{P}$$

$\rightsquigarrow$ mathematical manipulations, vector identities etc

But actually real physical charge accumulation

Saw this for slab. Can also understand angles





oblique cut.

same charge but

$A'\cos\theta = A$

$\sigma_b' = q/A'$

$= \frac{q\cos\theta}{A}$

$= P\cos\theta$

$= \vec{P}\cdot\hat{n}$

dipole moment

$P\cdot V = PAd = qd$

polarization per volume

$q = PA$

consistent $\sigma_b = \vec{P}\cdot\hat{n}$

$\cos\theta = 1$

induced dipole $\vec{p}$: uncharged conducting sphere has $\vec{p} = 0$ unless $\vec{E}_{ext}$ applied

permanent dipole $\vec{p}$

H_2O molecule

even in absence of $\vec{E}_{ext}$